determining a first indicia of an activity of a plurality of first test peptides from a first test peptide library;

selecting said first peptides using a space-filling design;

determining a relationship between the first indicia of the activity and at least two parameters of the plurality of first test peptides, wherein one parameter is a whole molecule parameter and an additional parameter is a sequence-specific parameter, and further wherein the length of said test peptides comprises no greater than twenty amino acids;

determining a test requirement relating to the measured first indicia; and

identifying at least one peptide from a second peptide library containing a plurality of second peptides which based on said relationship, are expected to provide an indicia of activity that satisfies said test requirement.

76. (Amended) The method of claim 74, wherein said step of determining a relationship comprises the step of determining $\hat{y}_i = f(x_{ij})$, where x_{ij} denotes a whole molecule parameter, i ranges from 1 to n where n represents the number of first test peptides in the plurality thereof, j ranges from 1 to d where d represents the number of whole molecule parameters, and $\hat{y}_i$ represents an estimate of the measured first indicia of the activity of the plurality of first test peptides.

81. (Twice Amended) The method of claim 74, wherein said determining first indicia step is preceded by the step of defining a first test peptide library by representing each of a plurality of groups of peptides as peptides sharing common global characteristics from a first peptide space as a respective candidate peptide.

82. (Twice Amended) The method of claim 81, further comprising the step of expanding less than all of the candidate peptides determined in said representing step into their constituent compound isomers using a space-filling design.

83. (Amended) The method of claim 74, wherein said whole molecule parameter is selected from the group consisting of total charge, molecular weight, isoelectric point and total dipole moment.

84. (Amended) The method of claim 74, wherein said whole molecule parameter is selected from the group consisting of total charge, molecular weight, isoelectric point, and total dipole moment, and further wherein said sequence-specific parameter is selected from the group consisting of isotropic surface area, electronic charge index, and hydrophobicity.

85. (Amended) The method of claim 74, wherein said sequence-specific parameter is selected from the group consisting of isotropic surface area, electronic charge index, and hydrophobicity.